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Scope of catalytic application of heterogeneous metal catalysts: Synthesis

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Abstract: Transition-metal catalysts, are foundational to Green Chemistry, influence energy storage, chemical production, and environmental solutions. Key metals include copper, which aids in alcohol oxidation and environmental cleaning; manganese, effective in reducing chromium(VI) and carbon dioxide; ruthenium, a cost-effective alternative for hydrogen evolution reactions; and iridium, with diverse roles from oxidation to enantioselective reactions. Additionally, rhodium-based catalysts play roles from C-H activation to hydroformylation of alkenes. Computational tools, like DFT, enhance understanding and optimization of these catalysts.

Key Words: Green chemistry, catalysts, oxidation, computational tool, eco-friendly.

Catalysis is a core to Green Chemistry, striving and designing for eco-friendly chemical processes. There are two main types of catalysis homogeneous and heterogeneous, homogeneous catalysis offers high efficiency but faces challenges like catalyst recovery, and heterogeneous, is known for environmental friendliness and easy catalyst recovery but sometimes lesser efficiency. Nano catalysis, a recent development, merges the benefits of both types, offering efficient reactions and easy recovery due to its increased surface area. The principles of Green Chemistry advocate for catalysts over stoichiometric reagents, reducing waste. Combining the activity of homogeneous catalysts with the recoverability of heterogeneous ones is vital for sustainable and economical chemical processes.

Transition metal catalysts: Transition-metal heterogeneous catalysts are pivotal in areas like energy storage, chemical manufacturing, and environmental solutions [11-12]. Their efficiency is influenced by atomic configurations around active sites. Understanding the structural stability of these active centers in different environments is essential for designing optimal catalysts [13]. Computational methods, like density functional theory (DFT) calculations, offer insights into these challenges without heavy experimental reliance [14]. Transition metals, central to the periodic table, can catalyze reactions either as metals or compounds, with examples like Ag(III), Cu(II), and Ni(IV) being notable oxidizing agents [15].

1. Copper catalyst: copper is a key component in various enzymes, such as galactose oxidase, and helps in the oxidation of alcohols.[16] Mark? et al. found that certain combinations involving copper enabled the oxidation of alcohols without disturbing other parts of molecules.[17] A study investigated the role of a specific form of copper in reducing chromium contaminants using citric acid and simulated sunlight.[18] Experiments were conducted to see if copper could aid in a chemical reaction known as the Ullmann-type, specifically for changing diethyl malonate.[19] Copper, when combined with graphene, proved effective in converting carbon dioxide into hydrogen. Other forms of copper catalysts are also used for environmental cleaning.[20] Bhanushali and his team transformed 1,4-butanediol into a compound called γ -butyrolactone using copper catalysts.[21] Mohamadpour et al. efficiently produced certain biologically active compounds using a form of copper, without needing solvents.[22] In essence, copper is a versatile catalyst, playing significant roles in various chemical transformations and environmental applications.

2. Manganese catalysts: Divalent manganese, or Mn(II), has been observed to have significant roles in various chemical processes: Studies used different techniques to find out that Mn(II) assists in the quick and effective reduction of the toxic chromium(VI) when oxalic acid is present in water.[23] Catalysts containing manganese are efficient in lowering carbon dioxide levels and removing nitric oxide, especially at cooler temperatures.[24] These Mn-based catalysts have also been applied in the oxidation of substances like 5-hydroxy methyl furfural and toluene.[25] Mn(II) catalyst was effectively used in the oxidation of 2-methylnaphthalene using hydrogen peroxide in an acetic acid environment.[26]

3. Ruthenium catalysts: Ruthenium is seen as a cost-effective alternative to platinum in the context of hydrogen evolution reactions.[27] Ruthenium-based catalysts have been successfully used in the hydrogenation of levulinic acid, oxidation of methyl bromide [28] hydrogenation of furfural [29], noticeable role is in stereo selective olefin metathesis reactions[30], Arylation, alkenylation, alkylation, and allylation [31]

4. Iridium catalysts: Iridium trichloride has been identified as a homogeneous catalyst that enhances the rate at which cerium(IV) oxidizes 3-phenyl propanal in an aqueous acidic medium.[32] Pandrala and colleagues demonstrated that Ir(III)-polypyridyl complexes are especially chemoselective catalysts for the reduction of aldehydes.[33] Complexes containing iridium and based on structures such as calix-[4]-pyrrole and porphyrin have been shown to be effective catalysts (both
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homogeneous and heterogeneous types). They demonstrate promising activity for the hydrogenation of levulinic acid, resulting in γ -valerolactone and 1,4-pentane-diol.[34] Iridium-based chiral catalysts have been harnessed for enantioselective reactions. A notable example is the enantioselective Nazarov cyclisation.[35] Iridium-based catalysts have a wide application range in organic synthesis. They play an integral role in the oxidation of various compounds, from primary and secondary alcohols to phenols, amines, phosphines, alkane, alkenes, and aromatic compounds.[36] Das and his team discovered that a chlorocomplex of Ir(III) serves as an efficient catalyst for the oxidation of D-glucose by N-bromophthalimide.[37]

Rhodium catalyst:

Rh(III), has been identified as a potent catalyst for the Ce(IV) oxidations of adjacent diols when in an aqueous sulfuric acid medium.[38] Highly regioselective methods have been developed that employ Rh(III) catalysis to achieve C-H activation, leading to the formation of isoindolin and dihydro isoquinolones derivatives.[39] An innovative method was crafted by Zhao and colleagues which facilitates the regio and stereo selective olefination of imidazoles in the presence of a cationic Rh(III) catalyst. Rhodium-based catalysts have shown efficiency in catalyzing the regioselective hydroformylation of lengthy alkenes.[40]

Conclusions: Transition metals catalysts play a critical role in the advancement of Green Chemistry, supporting eco-friendly and efficient chemical processes. Metals like Copper, manganese, ruthenium, iridium, and rhodium serve as vital catalysts. Each catalysts have unique applications ranging from oxidation reactions to complex organic syntheses. The advent of nano catalysis and computational methods like DFT amplifies our understanding and optimization of these catalysts. Their diverse roles in chemical transformations and environmental applications underline their importance.

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